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## 13. ABSTRACT (Maximum 200 words)

Work continued on order-parameter theories of two-phase continua. This work differs from past work in the introduction a balance law for microforces associated with the kinematics of the order parameter and the use of the second-law to develop constitutive equations.

A general framework for dynamical fracture is developed based on the notion of configurational forces in conjunction with a mechanical version of the second law. Here, as with other work done on this project, configurational forces are viewed as basic objects consistent with their own force balance. This balance yields a kinetic relation for the evolution of straight cracks. Kinking and curving of cracks is based on the requirement that the crack propagate in the direction that

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maximizes the energy dissipation. Explicit relations for the initial kink angle and the subsequent direction of propagation are given.

A continuum framework is developed for recrystallization. The driving force is the energy stored in dislocation substructures, characterized with the aid of a scalar measure, the dislocation content. A relation is obtained characterizing the efficiency with which dislocation substructure is eliminated by moving grain boundaries.

## FINAL TECHNICAL REPORT SUMMARY (1994-1997)

### STABILITY AND THERMAL INFLUENCES IN NONLINEAR CONTINUUM MECHANICS AND MATERIAL SCIENCE

Grant DAAH04-94-G-0224

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#### 1. Phase transitions

##### a. Configurational forces

The standard forces associated with continua arise as a response to the motion of material points. That additional, *configurational* forces may be needed to describe the internal structure of the material is clear from Eshelby's work on lattice defects and is intimated by Gibbs in his discussion of multiphase equilibria. These studies are statical, based on variational arguments, with configurational forces *defined* as derivatives of the energy. I take the different point of view that configurational forces should be viewed as basic primitive objects consistent with their own force balance. In [H1] I demonstrate the power of configurational force-balances in the study of phase transitions. In the standard theories of (i) Stefan-type solidification, (ii) interface motion neglecting bulk behavior, and (iii) solid-solid phase transitions an *extra* interface condition is needed: for (i), the extra condition is the classical Stefan condition, temperature equals melting temperature; for (ii), the condition is the motion-by-curvature equation; for (iii), (in the absence of interfacial stress) the condition is a kinetic relation of the type proposed by Truskinovsky, Abeyaratne, and Knowles. There are three compelling arguments in support of configurational forces: they provide a conceptual unification, as each of these extra conditions is a consequence of the configurational force-balance applied across the interface; they lead to new results, an example being a weak formulation of the supercooled Stefan problem; they provide a valuable tool in the framing of new theories.

##### b. Order-parameter theories

Work continued on order-parameter theories of two-phase continua. This work differs from past work in two aspects: the introduction a balance law for microforces associated with the kinematics

of the order parameter; the systematic use of the second-law to develop suitable constitutive equations. In particular, [H5] develops a unified framework for theories of Ginzburg-Landau and Cahn-Hilliard type, a framework that accounts for deformation and stress. [H3] (in collaboration with E. Fried, Penn State) develops a general phase-field theory of solidification. Balance laws for microforce and energy are used in conjunction with the second law to develop a general phase-field theory. A matched asymptotic analysis—appropriate to decreasing interface thickness—demonstrates the consonance of the theory with a general, thermodynamically consistent sharp-interface theory that accounts for anisotropic interfacial energy and entropy, interfacial tension and shear, and transition kinetics. [H4] (in collaboration with D. Polignone, Tennessee and J. Viñals, Florida State) develops a unified framework for coupled Navier-Stokes/Cahn-Hilliard equations using, as a basis, a balance law for microforces in conjunction with constitutive equations consistent with a mechanical version of the second law. As a numerical application of the theory, the kinetics of coarsening for a binary fluid in two space-dimensions is considered; these computations demonstrate a new effect in spinodal decomposition: the break-up and coalescence of particles.

#### **c. Diffusive phase transitions**

[H2] (in collaboration with P. Voorhees, Northwestern) develops a general thermodynamical description of an evolving interface. The theory represents a broad departure from theories based on classical nonequilibrium thermodynamics, as it does not presume a linear relationship between fluxes and forces, and it is not limited to small departures from equilibrium. Diffusion in both phases is considered, without an assumption of steady-state diffusion in bulk, the composition of material transferred across the interface is allowed to differ from the compositions of either phase, with solute drag included as a special case, and heat flow is allowed in both phases. As an application of the general theory, linearized interface conditions are developed.

#### **d. Evolution of interfacial curves and surfaces**

Phase interfaces and grain boundaries in crystalline materials often exhibit full-faceted (polygonal) shapes. Even so, there is almost no work toward analyzing the resulting free-boundary problems, chiefly because the lack of interface smoothness precludes standard treatments. A central tool in the analysis of smooth interface problems is comparison; it is central in the study of qualitative behavior and is a basic tool in establishing “viscosity-type” solutions. In [H6], written with Y. Giga (Hokkaido U.), a comparison theorem for crystalline evolution of a fully faceted curve in the plane is established. This result, the first of its kind, asserts that two evolving crystals one initially inside the other will remain in that configuration for all time, a result generalized in [H7] to three

space-dimensions. [H7], written with Giga and J. Matias (Lisbon U.), is based on fundamental work of Cahn and Hoffman.

## **2. Fracture**

[H9] and [H12], written with P. Podio-Guidugli (U. Rome), develops a framework for dynamical fracture, concentrating on the derivation of basic field equations that describe the motion of a crack tip in two space-dimensions. The theory is based on the notion of configurational forces in conjunction with a mechanical version of the second law. Unlike all previous discussions of fracture, configurational forces are viewed as basic objects consistent with their own force balance. This balance, when combined with suitable constitutive equations, yields a kinetic relation for the evolution of the straight cracks. An additional criterion is needed to discuss the kinking and curving of cracks; this is furnished by a requirement asserting that the crack propagate in the direction that maximizes the rate at which it dissipates energy. Explicit relations for the initial kink angle and the subsequent direction of propagation are given.

[H13], written with M. M. Schvartsman (Carnegie Mellon), extends the work on fracture to planar cracks in three-dimensional bodies. The line energy of the crack-tip curve is shown to serve as an impediment to crack growth, an effect especially important for small cracks.

## **3. Electromagnetic theory and superconductivity**

[H8] introduces a framework for electromagnetism with basic ingredients the electromagnetic potential, gauge invariance, an appropriate version of the second law, and constitutive equations. A central result is a derivation of Maxwell's equations as necessary and sufficient conditions for the gauge invariance of the second law. Using this union of thermomechanics and invariance, [H8] develops a general theory of superconductivity. What distinguishes this treatment from other macroscopic theories of superconductivity are the separation of basic physical laws from constitutive equations and the introduction of a balance law for complex microforces. This continues an approach based on the belief that fundamental physical laws involving energy should account for the work associated with each kinematical process. In the Ginzburg-Landau theory the macroscopic manifestation of the kinematics of superelectrons is the complex wavefunction  $\psi$ . In accord with this I assume that forces on superelectrons are characterized macroscopically by a complex microforce system that performs work when  $\psi$  undergoes change, and, what is most important, this microforce system is presumed consistent with a complex microforce balance. The final results consist of a hierarchy of coupled nonlinear partial differential equations, at various levels of generality, for the electromagnetic field and the superconducting electrons. The resulting theory is con-

sistent with, but far more general than, the classical Ginzburg-Landau theory.

#### **d. Recrystallization**

[H11], written with M. Lusk (Colorado School of Mines), develops a continuum framework for recrystallization. The driving force is the energy stored in dislocation substructures, characterized with the aid of a scalar measure, the dislocation content. Grain boundary kinetics are derived from a configurational force balance, a mechanical version of the second law, and suitable constitutive assumptions. A relation is obtained characterizing the efficiency with which dislocation substructure is eliminated by moving grain boundaries. Using a system of microforce balances, the sharp interface theory is shown to have a phase-field regularization that obviates the need to track grain boundaries. The sharp interface theory is recovered, via formal asymptotics, as a limiting case.

#### **Papers and reports which appeared under this contract**

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